Overcoming traceability challenge in air quality measurements by developing reference gas mixtures of CO_2 in a typical indoor/outdoor range for future relevant IoT technology applications

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ABSTRACT
High-resolution air quality monitoring using inexpensive sensor systems has attracted a lot of attention in the context of smart cities. However, in order to preserve metrological traceability, these systems must be regularly recalibrated. The necessity of quality control, dependability, and traceability of analytical data has received a lot of attention lately. IoT sensors can also be used to monitor the condition of equipment and ensure that it conforms with safety rules, given the rapid advancement of new technologies and their numerous everyday uses. Therefore, the primary motivation for our study endeavour was to provide reference gas mixtures to calibrate those sensors optimally in the future while keeping traceability to SI units, which is an important and demanding duty of gas standard laboratories at NMIs. Given the significance of metrological issues in the current context, the National Measurement and Calibration Center (SASO-NMCC) developed the methodology for preparing such primary standard gas mixtures (PSMs) through standardized gravimetric method in order to improve measurement capabilities and provide a level of confidence regarding greenhouse gas standards. Compatibility check, as per ISO 6143:2001, for the gas chromatography thermal conductivity detector (GC-TCD) with respect to the gravimetric assigned values with its associated combined uncertainty is also presented for each produced PSM. The relative expanded uncertainty of the carbon dioxide standard mixture, taking into account the contributions from verification analysis by GC-TCD, was less than 0.7 % for the prepared range of (0.00499 ± 0.00006) to (0.1996 ± 0.000424) mol/mol. This is comparable to the average of 0.25 % relative uncertainties presented on international standards mixtures.

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1. INTRODUCTION

In order to follow trends in atmospheric carbon dioxide (CO2) and greenhouse gases (GHGs) and to collect vital information on pollution levels and future orientations, metrological concepts must be applied. Determining the gaseous contaminants in the environment accurately and consistently is necessary for this. The detrimental impacts of rising CO2 concentrations in the atmosphere on people and the environment, including climate change and global warming, are the focus of the scientific community [1]–[7].

According to ISO 14065:2013, greenhouse gases are defined as gases that are part of the atmosphere that produce and absorb radiation at specific infrared wavelengths. There has to be more confidence in the achieved values of GHG mitigation reduction targets in order to track greenhouse gas sources and sinks and more accurately forecast climatic trends. Reliable GHG testing has to be developed for atmospheric measurements and local measurements of GHG emission components [8]–[11].

The scientific community is looking into the negative effects of rising atmospheric concentrations of CO_2, such as the greenhouse effect, which can cause climate change and contribute to global warming. The use of reference materials ensures the comparability and traceability of results acquired by other laboratories, promoting traceability across society and maintaining a global and uniform system of measurements across various laboratories [8]-[14].

As standards for measuring precision rise, there is a growing demand for measurements in various fields, including research, gas emissions, commerce, trade, medicine, ecology, and other human efforts. To guarantee the traceability of metrological measurements to SI units, it is essential to establish measuring standard equivalency, which uses units of measurement in cross-national comparisons. Traceability chains have a tree form during calibrations, adhering to ISO 17025 and ISO 17043.

Pollution, caused by industrialization, urbanization, population growth, and increased vehicle usage, disrupts the natural atmosphere and contributes to global warming. To combat this issue, implementing the Internet of Things (IoT) technologies to measure CO_2 emissions from public transports, and industries is crucial. The IoT is a future internet where devices, such as machines and sensors, exchange data without human intervention. The IoT-based CO_2 monitoring systems aim to monitor atmospheric and outdoor CO_2 rate. By collecting and analyzing large amounts of data, this system helps protect the environment and prevent global warming caused by CO_2 emissions as well as protecting the health of human beings in the indoor environments [15], [16].

CO_2 is a vital indicator of Indoor Air Quality (IAQ) and has a significant impact on public health. When CO2 levels above 1000 ppm, indoor air quality issues may arise. Real-time CO_2 concentration monitoring is crucial for identifying IAQ problems and taking prompt action within the building. The ability to create smart things with significant sensing and connecting capabilities is made feasible by ongoing technical advancements in a number of fields, including Ambient Assisted Living and the Internet of Things (IoT) [17],[18]. This urges the national metrology institutes (NMIs) to produce CRMs for the calibration of those intelligent systems and sensors network which is expected to complement with IoT applications to improve the quality of life, that emphasize the crucial role played by metrology in our daily life. This presents one of the objectives of this work.

In this work, an in-house preparation scheme of reference gas mixtures of CO_2 in N_2 as primary standard mixtures (PSMs) cylinders using the gravimetric method is presented, the method complies with ISO 6142, and uses a validated gas chromatography thermal conductivity detector (GC-TCD) to confirm the mole fraction of the gas mixtures created gravimetrically. Mid- and long-term evaluations show that the produced concentrations are reproducible. For GC verification, eight certified reference materials (CRMs) in varying concentrations were used to ensure metrological traceability of the measurement outcomes to SI units. Based on the result evaluation under given criteria, it can be concluded that the GC-TCD method is reliable and suitable for determining high levels of CO_2 in N_2 matrix.

2. GRAVIMETRY

2.1. Introduction

One basic methodology that can be utilized for the preparation of primary gas mixtures in high pressure cylinders as well as the development of primary reference standards is gravimetry. Direct traceability to mass standards and the purity of the parent gases are provided by gravimetry. There are two steps in the preparation process at SASO-NMCC: First, initialization and conditioning; second, weighing. The gas cylinder is evacuated and heated for a few hours during the conditioning process, after which it is filled with matrix gas (often nitrogen or synthetic air). Usually, the conditioning cycle is carried out three times. Since the presence of contaminants would cause the gas mixture to degrade quickly, the conditioning stage seeks to remove pollutants from the interior walls of the cylinder.

2.2. Gravimetric preparation method and associated uncertainty in the measured mole fractions

ISO 6142 and ISO 6143 outline the main sources of uncertainty for reference materials, including raw material purity, environmental conditions, equipment calibration, measurement and volumetric errors, stability and homogeneity, interaction with container materials, and method of preparation. Impurities in raw materials, environmental conditions, equipment calibration, measurement and volumetric errors, stability and homogeneity, interaction with container materials, and method of preparation can all contribute to the uncertainty in reference materials.

Based on the calculation formula stated in the mentioned standards [11]-[13], three categories of sources of uncertainty can be distinguished:
- parent gases CO_2 and N_2 purity (see Table 1)
- parent gases CO_2 and N_2 weight and
- molar masses of CO_2 and N_2.

Below is an explanation of how each uncertainty component was calculated in detail in Table 2.

In summary, the uncertainty components in the used gravimetric method: (A) Purity uncertainty of parent gases, (B)

Table 1. Purity table of cylinder PSM-01.

Component	Symbol	Mass fraction	Mole fraction	Uncertainty (mol/mol)
Carbon monoxide	CO	$2.4801 \cdot 10^{-7}$	$2.4875 \cdot 10^{-7}$	$1.3727 \cdot 10^{-7}$
Carbon dioxide	CO_2	$7.8304 \cdot 10^{-3}$	$4.9985 \cdot 10^{-3}$	$2.3193 \cdot 10^{-7}$
Total hydrocarbon	C_xH_y	$3.9044 \cdot 10^{-7}$	$2.4875 \cdot 10^{-7}$	$1.3727 \cdot 10^{-7}$
Water	H_2O	$7.9833 \cdot 10^{-7}$	$1.2449 \cdot 10^{-6}$	$5.6772 \cdot 10^{-7}$
Nitrogen	N_2	$9.9217 \cdot 10^{-1}$	$9.9500 \cdot 10^{-1}$	$1.5119 \cdot 10^{-6}$
Oxygen	O_2	$2.9756 \cdot 10^{-6}$	$2.6125 \cdot 10^{-6}$	$1.3746 \cdot 10^{-6}$

Table 2. Uncertainty budget for mole fraction of PSM-1 of CO_2.

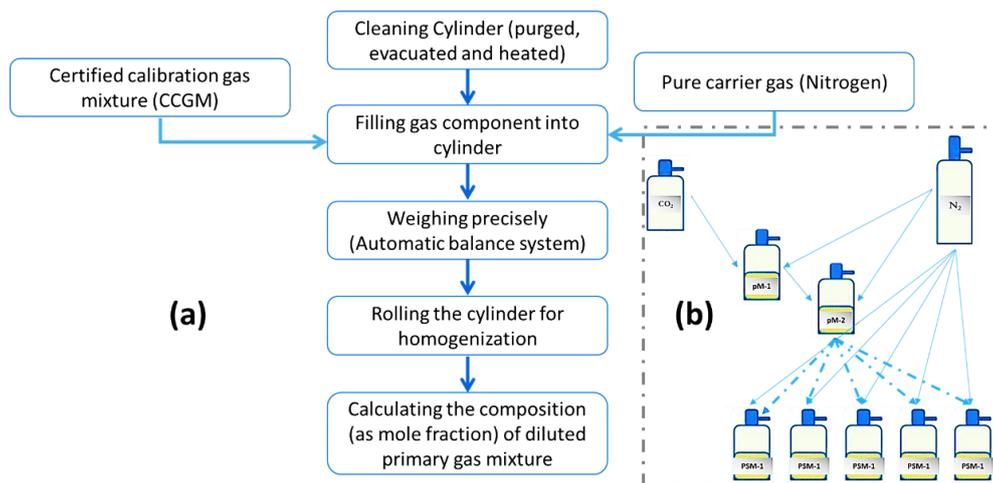| Source	Standard uncertainty, $u(x_i)$	Unit	Uncertainty contribution, $c_i u_i$
Mass of CO_2	$5.97 \cdot 10^{-5}$	g	$5.27 \cdot 10^{-7}$
Molar mass of CO_2	$9.40 \cdot 10^{-6}$	g/mol	$5.36 \cdot 10^{-7}$
Purity of CO_2	$5.75 \cdot 10^{-8}$	mol/mol	$2.32 \cdot 10^{-7}$
Mass of N_2	$5.97 \cdot 10^{-5}$	g	$2.07 \cdot 10^{-7}$
Molar mass of N_2	$2.50 \cdot 10^{-6}$	g/mol	$1.42 \cdot 10^{-7}$
Purity of N_2	$1.80 \cdot 10^{-8}$	mol/mol	$1.66 \cdot 10^{-8}$
Combined standard uncertainty, u_c		**2.32E-07**	**mol/mol**

Figure 1. Scheme for the primary gas mixture's gravimetric dilution, where "a" presents a simplified flow chart and "b" visualizes the stages of the production, with pMs denote the pre-mixtures [20].

produced; next, this mixture should be diluted to produce lower concentrations with traceability obtained. Figure 1a and Figure 1b simplify this production plan [19].

The parent gases that were used for the gravimetric dilution of primary gas mixtures is the pure CO_2 (99.8%) and N_2 (99.9999%) gases supplied by LINDE-SIGAS, Germany, which in terms of their purities, are certified reference gas mixes (CRMs). Air Liquide, located in the Netherlands, provided the 5-L aluminium cylinders that were used to fill them with gas mixtures.

Uncertainty in weighing of the parent CO_2 and N_2 gases; which includes balance certificate uncertainty, balance repeatability uncertainty, buoyancy uncertainty and residual gas uncertainty, (C) Uncertainty of molar masses of both CO_2 and N_2.

The evaluated combined standard uncertainties associated with each PSM are used in Table 4 for computability analysis. The corresponding gravimetric preparation uncertainties of all the prepared PSMs are all stated in the Table.

3. MATERIALS AND METHOD

3.1. Materials

In order to help stabilize the prepared gas's concentration, pure gases with their molecules dispersed among inert nitrogen gas molecules or pure air molecules are used to create gas mixture reference materials. It is best to develop the CRMs in two stages: first, a high-concentration mixture with traceability should be

Figure 2. Photograph of evacuation system and its schematic.

3.2. Apparatus

Equipment comprises the evacuation system, filling system, weighing system, balance, homogenizer system, and Gas Chromatography system (GC-TCD) for verification analysis. The Evacuation System (PFEIFFER, model: HiCUBE) is used to evacuate the sample cylinder and to purge used and new cylinder. The Evacuation System is built up with a pumping station with maximum four cylinder-connections by changing the existing valve locations. List of the used equipment and detailed specifications shown in detail elsewhere [19].

3.3. Method

In-house preparation method of the primary gas mixtures was done according to "ISO 6142-1: Gas analysis – preparation of calibration gas mixtures" [2]. Steps of the method, as per the standard, can be summarised as follows:

1 - calculate masses and uncertainties,
2 - prepare composition including filling sequence,
3 - perform purity analysis,
4 - prepare the mixture and determine masses,
5 - determine molar masses, calculate mixture composition and uncertainty,
6 - homogenise the mixture,
7 - perform verification, and
8 - if verification result is fulfilling the compatibility condition stated in ISO 6143 (refer to Equation (1) and Table 3), then report the results of concentrations and associated uncertainties (certificate).

To show the verification process in visible figures, carbon dioxide gas with a concentration of $(0.049925694 \pm 0.0000659)$ mol/mol with nitrogen as balance is presented as an example of the verification process (refer to Table 1 to Table 4). This example mixture is denoted as "PSM-03". The method used for the production process, as shown in Figure 1, is broken down into a number of steps, beginning with completely emptying the cylinder (see Figure 2). To do this, the cylinder is connected to a vacuum device for a period of 12 hours, during which time all impurities are removed. When the cylinder is completely empty, the pressure indicator changes to 1×10^{-7}, signifying that the preparation process is complete [19].

Following discharge, the procedure of calculating the quantity based on the prepared target concentration using the weighing equipment commences. By contrasting the sample cylinder with
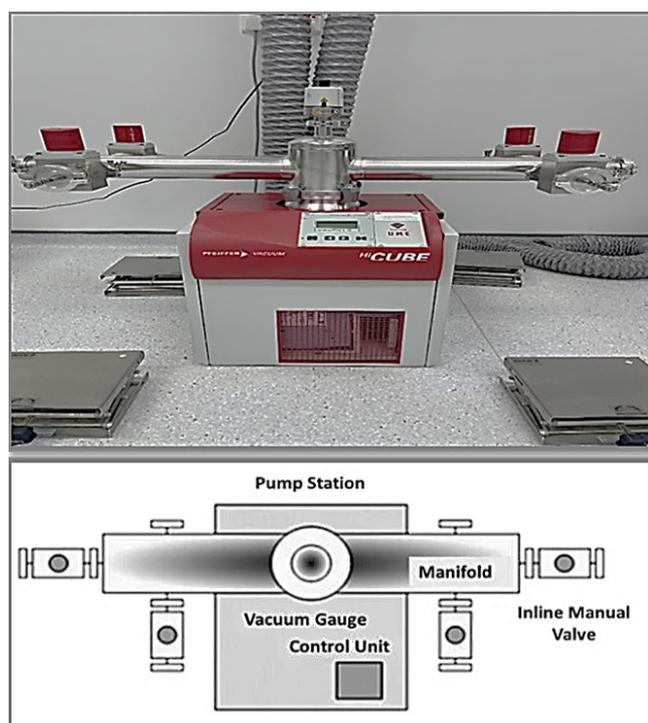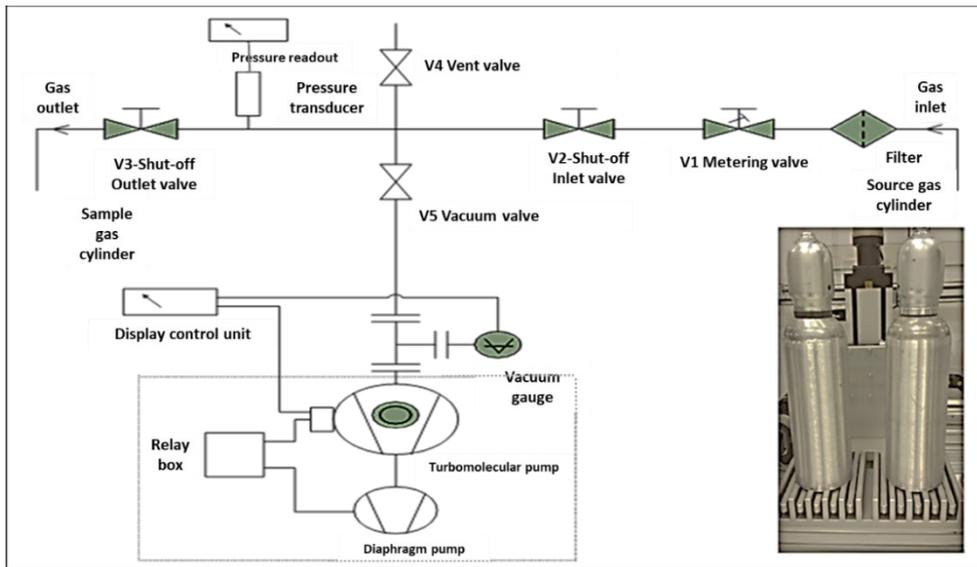
Figure 3. Schematic of filling system, with photo of the automatically weighing system.

have been verified by GC–TCD in accordance with ISO 6143 (see Figure 4). For production and certification of the developed five primary mixtures, we used eight CRMs for verification process with concentration range $(0.0100 - 0.100000)$ (mol/mol) to ensure the traceability of the measurements. The set of eight CRMs produced by Turkish Institute of Metrology (TUBITAK-UME) been used for production and verification processes. So that the concentrations of the unknown samples were in the same range. Each CRM was injected 10 times and the prepared gas mixture samples were injected 10 times per each. The analysis develops set of chromatograms corresponding to each sample (see Figure 5). The average was calculated, and the calibration curve was obtained by plotting the CRM concentration (x) against the corresponding peak area (y). The concluded calibration curve is shown in Figure 6, which shows a linear behavior with the equation and R^2 figure shown on the graph. Coefficient of determination "R^2" equals one as shown. The standard uncertainty $u(y_i)$ was calculated as per ISO 6143 standard and the results are shown in Table 3.

the reference cylinder, the device is intended to automatically weigh the gas cylinder (Figure 3).

The ideal gas law $P\ V = n\ R\ T$ is the foundation of the system. The maximum weight and volume permitted for a cylinder are also shown in Figure 3, where the permitted weight varies from (1 mg to 10 100 g) and the size of its cylinder is (5 L).

After completing the weighing process in accordance with the ideal gas law, which provides us with the required weight to attain the correct concentrations, we begin the filling process using a filling system. By applying the filling mechanism with volumes of pure gas or gas mixtures, the primary gas mixtures are produced. The system can fill the 5L-cylinders in accordance with ISO Standard 6142-2001[11], Every gas flow line is composed of electro-polished stainless steel that can withstand pressures up to 200 bar. The system can evacuate all lines, from pure gases to sample cylinders, to a vacuum of about 1×10^{-6} mbar. The schematic diagram of the filling mechanism is shown in Figure 3 [19].The purpose of the mixing stage is to enhance the homogeneity between the gases, which is a prerequisite of the reference material when using a mixing device, after the quantity, filling, and gas concentrations have been determined. The cylinder homogenization system, shown in [19], is made up of three rollers that the cylinder is placed on and a control panel that modifies the rollers' rotational orientations and speeds. The roller at the system's core is turned by the motor, and each roller on the system's outside edges moves independently of the others. Two cylinders can be mixed at once. The primary gas mixtures of CO_2 in N_2 prepared gravimetrically according to ISO 6142

Comparability criteria as per ISO 6143 can be stated as follows:

$$|x_{\text{grav}} - x_{\text{GC-anal}}| \leq 2\sqrt{u(x_{\text{grav}})^2 + u(x_{\text{GC-anal}})^2}, \qquad (1)$$

in this in-equality, x_{grav} and $x_{\text{GC-anal}}$ denote the calculated mol fraction by gravimetric method scheme and the concluded from the GC analysis, respectively, and $u(x_{\text{grav}})$ and $u(x_{\text{GC-anal}})$ denote the standard uncertainties of these quantities. Where, both x_{grav} and $u(x_{\text{grav}})$ can be directly calculated using equations (3) and (4) in [11].

4. VERIFICATION OF GAS MIXTURE COMPOSITION USING GC-TCD

Gas metrology relies heavily on gas chromatography (GC) and other chromatographic techniques to separate compounds of analytical relevance. The principal method for analyzing fire
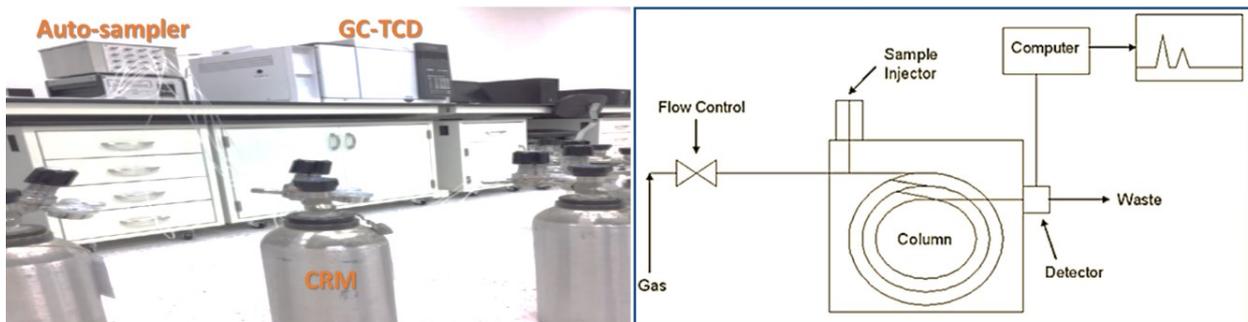

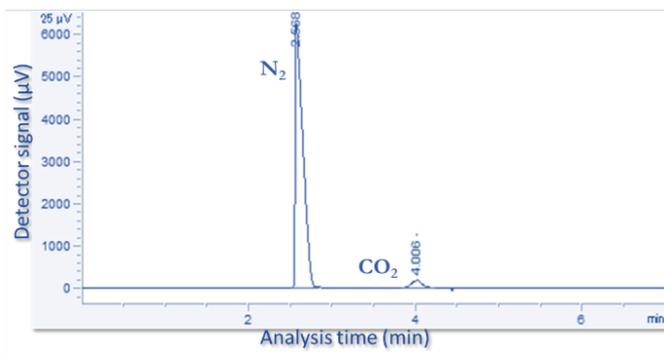Figure 4. Gas Chromatography (GC) real photo (left) and schematic (right).

Figure 5. Typical chromatogram of gaseous mixture, showing the peaks of interest (one selected example of the analyzed sample PSMs).

remains is gas chromatography (GC). Petroleum products are typically utilized as fire accelerants, and the peak patterns from the GC analysis can be used to determine the kind of product (such as gasoline) that was used in the fire. Drug analysis was one of the first applications of GC in forensic research. With GC, a variety of gases may be distinguished and measured. Additionally, in medicine, once the appropriate extraction procedures have been completed, GC can also be used to test blood and other bodily fluids for the presence of medicines and poisons. In gas composition analysis (GC), a separation column composed of glass, fused silica, or metal tubing is utilized. The mobile phase travels through the separation column and toward a detector, much like in other types of chromatography. In GC, an inert gas such as hydrogen, helium, or nitrogen is employed as the mobile phase. The term "mobile phase" usually refers to a carrier gas, which is responsible for carrying each component toward the detector when a combination of substances is introduced at the column intake.

The versatile thermal conductivity detector (TCD) is capable of detecting a wide range of substances, including air, hydrogen, carbon monoxide, nitrogen, sulfur oxide, and inorganic gases. In gas chromatography, thermal conductivity (TCD) is a frequently employed detector. Two parallel tubes, one holding gas and the other heating coils, are how TCD operates. By comparing the rate of heat loss from the heating coils into the gas, the gases are analyzed. Typically, the substance to be evaluated is passed through one tube, which contains a reference gas. By applying this theory, a TCD measures variations in the column effluent's thermal conductivity and contrasts it with a carrier gas reference flow. The thermal conductivity of most compounds is significantly lower than that of helium or hydrogen, which are popular carrier gases. As a result, a measurable signal is generated, and the thermal conductivity of the effluent is decreased when an analyte elutes from the column. Although helium has long been the preferred carrier gas, recently hydrogen has been used as alternative for the GC-TCD as laboratory trends shift.

Verification data are collected and concluded via Xgenline (v1.1) software [21].

5. UNCERTAINTY ANALYSIS

The uncertainty estimation of the measurement of CO_2 concentration was carried out using the bottom-up approach based on EURACHEM/CITAC Guide CG4 [20].

The potential sources of uncertainty and how they might affect the value of the measurand are identified and analyzed.

In addition, there are many factors affecting the GC analysis, which can be summarized in many categories as follows [20], [22]:

A Result of analysis: carrier gas flow rate, column temperature, sample size, and split ratio.
B Peak area: carrier gas flow rate, baseline drift, noise, and peak resolution, among others.
C Peak height: column temperature, detector temperature, integrator settings, and repeatability of sample injection, among others.
D Split injection: injector liner, injector temperature, split ratio, among others.
E TCD: detector temperature, wire temperature, carrier gas flow rate.

The combined standard uncertainty u_c

Taking into account the previously mentioned factors, which can be categorized into type A and Type B uncertainty, as per [21]-[23]. Since the standard uncertainties are of different units, the combined standard uncertainty, u_c is calculated as ratios and the resulting ratio is multiplied by the sample gas concentration, C_0 as shown in equation (2).

$$u_c = C_0 \sqrt{\left(\frac{u_{CRM}}{C_{CRM}}\right)^2 + \left(\frac{u_{PACRM}}{PA_{CRM}}\right)^2 + \left(\frac{u_{PASample}}{PA_{Sample}}\right)^2}, \qquad (2)$$

where, u_{CRM} is the certified uncertainty of the C_{CRM}, PA_{CRM} is the peak area of the CRM and u_{PACRM} is the associated uncertainty with peak area (both stated in Table 4). Similarly, PA_{Sample} and $u_{PASample}$ are the peak area and associated uncertainty of the analysis of the prepared PSMs (both stated in Table 1 and Table 3). Table 5 reports a comparison between the values of PMSs obtained by GC and by gravimetry. Main uncertainty components considered in equation (2). Some of those components includes many sources of uncertainty (e.g. those stated in the uncertainty categories "A to E" above. While the detailed description of each and every component is beyond the scope of this work.

The expanded uncertainty at 95 % confidence level ($k = 2$) of five PSMs was calculated in the range of 0.002 to 0.10 relative to the mole fraction of final gas mixtures from the estimation of uncertainty for the gravimetric dilution of calibration gas mixtures (CO_2 in N_2 Balance). The uncertainty budget of the GC-TCD analysis for the prepared primary standard mixture "PSM-03" shown in Table 4.

The combined uncertainty associated with gravimetric preparation are concluded in Table 5, but the full uncertainty analysis in gravimetric preparation, including cause-and-effect diagram, the compatibility analysis in accordance with ISO 6143 as well as the long-term stability are beyond the scope of this paper; for in-progress subsequent publication related to carbon dioxide in atmospheric synthetic gas mixture.

6. RESULTS AND DISCUSSIONS

In this work, we prepared five PSMs with different concentrations, using the CRMs (certified gas mixtures) using the scheme described in section 2. Table 3 presents peak areas of the PSMs and the relative standard deviation % RSD figures for showing the precision of the measurement results. Results shown in Table 3 reflects the reproducibility and high-precision of the method with the "%RSD" presented to indicate the precision-suitability of the measurement results. The concentration range

Table 3. Peak areas of the PSMs and the % RSD figures for showing the precision of the measurement results.

	PSM-01	PSM-02	PSM-03	PSM-04	PSM-05
	245.76	497.50	2510.77	5013.98	10018.45
	245.90	497.56	2510.64	5014.96	10016.79
	245.87	497.72	2510.42	5016.41	10018.50
	245.78	497.59	2510.05	5016.65	10020.19
	245.88	497.68	2510.26	5015.58	10020.98
Peak Area	245.94	497.92	2509.17	5016.78	10020.55
	245.90	497.80	2509.31	5018.45	10021.59
	246.01	497.82	2509.11	5019.37	10022.94
	245.92	497.54	2509.62	5020.60	10022.69
	246.06	497.67	2509.68	5022.83	10023.02
	246.09	497.75	2510.14	5022.11	10022.59
Average, y	245.836	497.597	2509.995	5017.974	10019.756
stdev	0.186	0.224	0.648	2.936	3.120
RSD, %	0.076	0.045	0.026	0.059	0.031
$u(y)$	0.048	0.060	0.173	0.885	0.865
$u(y)$, %	0.020	0.012	0.007	0.018	0.009

Table 4. Verification of gas mixture composition using GC (for PSM-03).

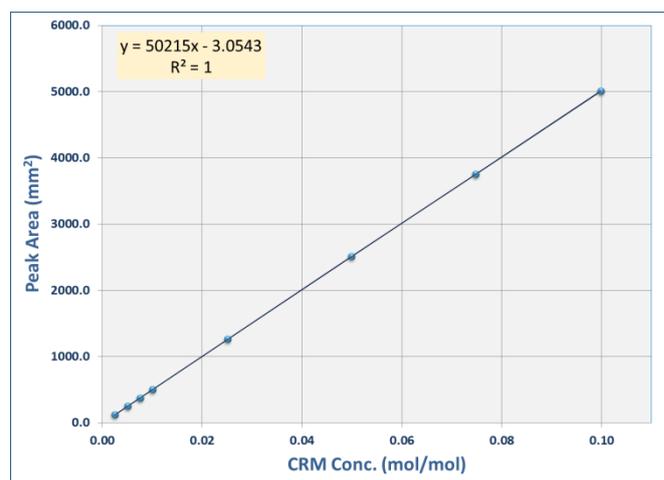|	x-values	Uncertainties Associated with x-values	y-values	Uncertainties associated with y-values
CRM-01	$2.50 \cdot 10^{-3}$	$2.50 \cdot 10^{-6}$	119.762333	0.119
CRM-02	$5.00 \cdot 10^{-3}$	$5.00 \cdot 10^{-6}$	245.968400	0.043
CRM-03	$7.50 \cdot 10^{-3}$	$7.50 \cdot 10^{-6}$	371.968000	0.144
CRM-04	$1.00 \cdot 10^{-2}$	$1.00 \cdot 10^{-5}$	498.400143	0.090
PSM-03	$4.99 \cdot 10^{-2}$	$3.30 \cdot 10^{-5}$	2509.995143	0.173
CRM-05	$2.51 \cdot 10^{-2}$	$2.51 \cdot 10^{-5}$	1259.240500	0.513
CRM-06	$4.98 \cdot 10^{-2}$	$4.98 \cdot 10^{-5}$	2508.130923	0.384
CRM-07	$7.47 \cdot 10^{-2}$	$7.48 \cdot 10^{-5}$	3749.651231	0.358
CRM-08	$9.99 \cdot 10^{-2}$	$9.99 \cdot 10^{-5}$	5007.491400	1.170

Figure 6. Concluded calibration curve showing the relationship between the response of the device (GC) and the concentrations of the reference materials (CRMs).

7. CONCLUSIONS

This paper discusses recent developments in the gravimetric production of primary standard gas mixtures of carbon dioxide in N₂ at SASO-NMCC, aiming to provide traceability and confidence in air quality monitoring research and analysis. Primary standard mixtures were prepared in accordance with ISO 6142:2015 and ISO 6143:2001 and are planned to undergo ISO 17034:2016 certification. The materials are prepared in-house and used as working standards in the lab to transfer traceability from parent CRMs to customers' DUTs. An approach for evaluating measurement uncertainty and validating the procedure is presented, with the estimated GC method being confirmed for measuring CO_2 volume fraction in N2 gas mixtures. The study highlights the importance of thoroughly characterizing the analytical system before beginning any analysis. The internal consistency of the prepared gas mixtures was verified using gas chromatography and thermal conductivity detector (GC-TCD), and the developed calibration gas mixtures showed satisfactory results for CO_2 components with comparable uncertainty levels to other standards laboratories.

The results showed that good internal consistency was achieved between the gravimetrical and GC's verification values, having linear regression coefficient $R^2 \geq 0.999$. The preliminary t-test result has shown that CO_2 has reasonably good short-term stability. In conclusion, the developed calibration gas mixtures at a typical concentration range have shown satisfying results for CO_2 component with comparable uncertainty levels to the other standards laboratories.

of the produced PSMs is 0.004995501 to 0.199585229 mol/mol. The verification process using GC-TCD had been done as shown in Table 4 and compatibility analysis in Table 5. The full uncertainty budget drawn in Table 6. The summary of the prepared concentrations and the associated uncertainties shown in Table 7. The produced reference PSMs are used for the calibration of the customers' artefacts with transferring the traceability of the relevant calibration activities and IoT activities.

Table 5. Compatibility analysis of the produced PSMs based on ISO 6143 criteria.

	y-values	Uncertainties associated with y-values	C analysis	u analysis	C gravimetric	u gravimetric	Compatibility test
PSM-01	245.8357333	0.048	0.004995501	$2.98 \cdot 10^{-6}$	0.004998	$2.32 \cdot 10^{-7}$	PASS
PSM-02	497.5968571	0.060	0.009997811	$3.93 \cdot 10^{-6}$	0.009998	$2.88 \cdot 10^{-7}$	PASS
PSM-03	2509.995143	0.173	0.049925694	$3.30 \cdot 10^{-5}$	0.049967	$1.46 \cdot 10^{-6}$	PASS
PSM-04	5017.974273	0.885	0.099824869	$5.60 \cdot 10^{-5}$	0.099889	$2.45 \cdot 10^{-6}$	PASS
PSM-05	10019.75554	0.865	0.199585229	$2.12 \cdot 10^{-4}$	0.199919	$4.46 \cdot 10^{-6}$	PASS

Table 6. Uncertainty budget of the GC-TCD measurements of one of the prepared PSM-03.

Cylinder	Source	X	u(X)	Unit	u(X) / X
		119.7623333	0.119191108		0.00099523
		245.9684	0.043327414		0.00017615
		371.968	0.144008242		0.000387152
		498.4001429	0.0901793		0.000180938
PSM266406	*CRM*	1259.2405	0.512830786	mol/mol	0.000407254
		2508.130923	0.383998706		0.000153102
		3749.651231	0.357844189		9.5434E-05
		5007.4914	1.169221519		0.000233494
		u_c(CRM)			**0.001207088**
		Y	u(y)		u(y) / y
		504.000000	0.206000		0.0010000
		504.000000	0.419000		0.0010000
		1010.000000	1.020000		0.0010003
Peak Area (R)		1260.000000	0.362000	mm^2	0.0010000
		2520.000000	1.290000		0.0010000
		2520.000000	1.490000		0.0010000
		3780.000000	1.200000		0.0010001
		5050.000000	1.660000		0.0009998
		u_c(PA(R))			**0.002828498**
Peak Area (S)		2509.995143	0.173305988	mm^2	**0.000069**
C_0 (mol/mol)		0.04993			
u_c		0.00308			
$C_0 \times u_c$		0.00015		mol/mol	
U_{Exp}		0.00031		mol/mol	
U_{Exp} %		0.62		%	

Table 7. Summary of the prepared PSMs concentrations and associated uncertainties.

PSM Code	Concentration in mol / mol	Expanded uncertainty in mol/mol
PSM-1	0.004995501	0.0000597
PSM-2	0.009997811	0.0000787
PSM-3	0.049925694	0.0000659
PSM-4	0.099824869	0.000112
PSM-5	0.199585229	0.000424

The gas industry can improve material traceability by utilizing IoT technologies to track supply and equipment movement in real-time, optimize logistics, and ensure timely delivery. However, integrating IoT technology in the oil and gas sector presents challenges, including compatibility with existing systems and procedures. Project managers, suppliers, logistics companies, and stakeholders must coordinate to ensure optimal calibration of sensors and maintain traceability to SI units.

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